Sandia National Laboratories

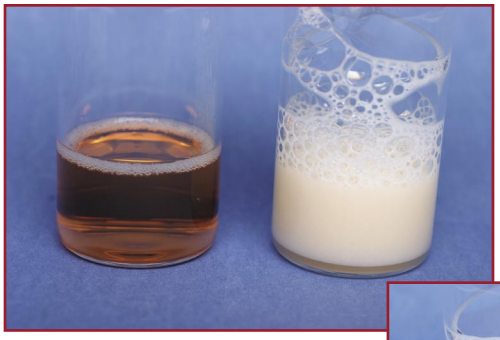
Fact Sheet

Thermally Cleavable Surfactants based on Diels-Alder Chemistry:

Useful in a variety of applications that call for control of surface tension or require non-invasive removal techniques

Background

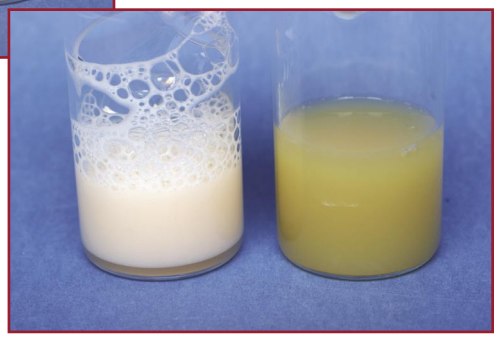
Surfactants are ubiquitous in commercial, industrial, and household applications. By their very nature, surfactants are typically very difficult to remove from any system in which they are employed. The concept of cleavable surfactants has recently been the area of significant research interest to help alleviate this problem of surfactant removal. Cleavable surfactants that are commercially available usually require the introduction of an acid and/or base to hydrolytically cleave the surfactants into fragments in order to eliminate them. These hydrolytically cleavable surfactants have found a niche application in the realm of biomedical diagnostic sample preparation, where a surfactant can be utilized to lyse a cell and then be removed before analyzing the sample components through mass spectrometry or other analytical techniques. The major drawback to this approach is that it requires the *invasive* introduction of another component into the system that may necessitate post-treatment of the system to achieve acceptable downstream processing conditions (i.e., pH).



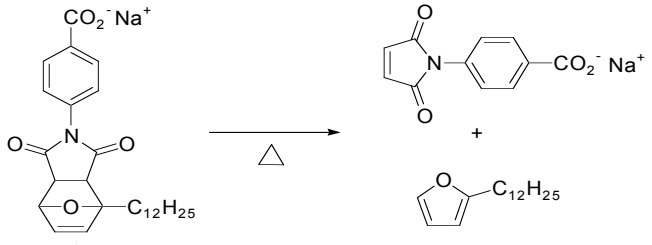
Left, a cleavable surfactant in aqueous solution dissolves an oil-soluble dye. Right, that same system forms an emulsion when oil is added.

Solution

Sandia National Laboratories is the world's leader in the development and introduction of thermally labile Diels-Alder adducts into molecules and materials that allow for non-invasive degradation and removal. Examples include the production of thermally responsive encapsulants, foams and adhesives, as well as macromolecules which reversibly self-assemble through covalent chemistry. Researchers have now developed a new class of patent-pending cleavable Diels-Alder based surfactants that degrade through simple thermal treatments. These are the first examples of surfactants that can be



Left, an intact emulsion. Right, the emulsion is broken after the cleavable surfactant is degraded by heating.



Example of cleavable anionic surfactant.

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thermally degraded in a benign manner. Five anionic surfactants are available which incorporate hydrophilic and hydrophobic segments which covalently degrade at elevated temperatures. These surfactants behave like classical surface active agents, and form micelles after reaching certain concentrations in water. Upon cleavage, the surfactants lose all surface-active behavior.

Application

Commercially available cleavable surfactants would enable industrial practices where it is desirable to diminish foaming or surface-active properties over time, in drug delivery, and where biodegradability is a primary concern. They could prove useful in such diverse fields as textile processing, electronics fabrication, sample management, wastewater processing, cleavable phase transfer reagents, and as removable templates for the construction of microporous zeolitic materials as well as templates of complex hierarchical materials.

Table of Surfactant Properties

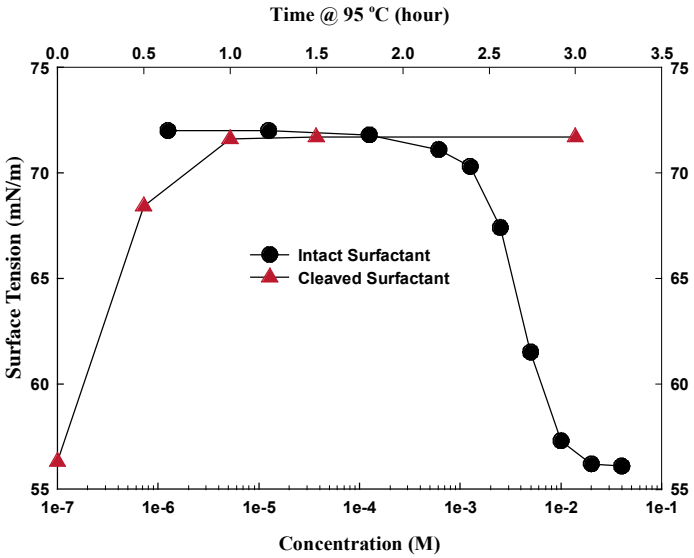
Headgroup	CMC (mM)	C_{20} (mM)	Γ (mol/cm2)
Phenolate	2.5	1.8	4.8×10^{-10}
Sulfonate	5.1	6.2	3.6×10^{-10}
Carboxylate	9.3	n/a	2.9×10^{-10}

Benefits

Stable in aqueous solutions, these surfactants possess good wetting characteristics. When exposed to elevated temperatures (> 50 °C), they spontaneously degrade, yielding non-surface active hydrophilic and hydrophobic fragments. All surfactants are produced in high yield and purity and offer an attractive alternative to other costly or invasive methods of surfactant removal.

Status

Partners who might wish to further develop these materials are welcome to contact Sandia/California's Business Development Support Department.



This graph shows the typical surface tension properties (black) and cleaving properties (red) of an anionic Diels-Alder surfactant.

References

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Learn more at: http://www.ca.sandia.gov

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